201-15012B

I U C L I D
Data Set

EP-306

Existing Chemical	:	ID: 68915-38-8
CAS No.	:	68915-38-8
TSCA Name	:	Cyclohexane, oxidized, aq. ext.

Producer related part

Company	:	BASF Corporation
Creation date	:	12.12.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	12.12.2003
Memo	:	
Printing date	:	30.12.2003
Revision date	:	
Date of last update	:	30.12.2003
Number of pages	:	18
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	manufacturer
Name	:	BASF Corporation
Contact person	:	
Date	:	
Street	:	3000 Continental Drive
Town	:	Mt. Olive, NJ 07828-1234
Country	:	
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

16.12.2003

1.2 SYNONYMS AND TRADENAMES

EP-306 Acid Water
COP Acid Water
Dicarboxylic Acid Solution
Dicarbonsaeure Loesung A. Ber. Trocken
Dicarbonsaeure Loesung L. Ber. Trocken
Abstreifsaeure

2.1 MELTING POINT

Value	:	35 – 45 °C
Method	:	Determined via unknown method by BASF Corporation on product
Year	:	
GLP	:	
Test substance	:	EP-306 Acid Water
Remark	:	
Reliability	:	(2) valid with restrictions

26.12.2003 (1)

Value	:	-6 °C
Method	:	Determined via unknown method by BASF AG on product
Year	:	
GLP	:	
Test substance	:	Dicarbonsaeure Loesung A. Ber. Trocken
Remark	:	Solidification temperature
Reliability	:	(2) valid with restrictions

26.12.2003 (2)

2.2 BOILING POINT

Value	:	ca. 101 °C at 1013 hPa
Decomposition	:	
Method	:	Determined via unknown method by BASF AG on product
Year	:	
GLP	:	
Test substance	:	Dicarbonsaeure Loesung A. Ber. Trocken
Remark	:	Initial value
Reliability	:	(2) valid with restrictions

26.12.2003 (2)

2.3 DENSITY

Type	:	Density
Value	:	= 1.04 g/cm³ at 50 °C
Remark	:	Measured value for typical product
Test substance	:	EP-306 Acid Water
Reliability	:	(2) valid with restrictions

26.12.2003 (1)

Type	:	Density
Value	:	= 1.06 g/cm³ at 45 °C
Test substance	:	Dicarbonsaeure Loesung A. Ber. Trocken
Remark	:	Measured value for typical product
Reliability	:	(2) valid with restrictions

26.12.2003 (2)

2.4 VAPOUR PRESSURE

Value	:	77 hPa at 40 °C
Decomposition	:	
Method	:	Determined via unknown method by BASF AG on product
Year	:	
GLP	:	
Test substance	:	Dicarbonsaeure Loesung A. Ber. Trocken
Remark	:	Initial value
Reliability	:	(2) valid with restrictions

26.12.2003 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	-0.59 to 1.92
pH value	:	-
Method	:	other (calculated): EPI Suite (v3.10)
Year	:	
GLP	:	
Test substance	:	

Method : The Ko/w of each component was calculated with EPI Suite based on its CAS No. The table below provides a summary of the Ko/w values for each component and indicates whether the value was an experimental value listed in EPI Suite (exp) or a value calculated by EPI Suite (cal).

Result :

EP-306 Component	Log Ko/w
Formic Acid	-0.54 (exp)
Acetic Acid	-0.17 (exp)
Propionic Acid	0.33 (exp)
Butyric Acid	0.79 (exp)
Valeric Acid	1.39 (exp)
Caproic Acid	1.92 (exp)
Succinic Acid	-0.59 (exp)
Glutaric Acid	-0.29 (exp)
Adipic Acid	0.08 (exp)
6-Hydroxycaproic Acid	0.59 (cal)
Cyclohexanol	1.23 (exp)
Cyclohexanone	0.81 (exp)
Cyclohexyl Hydroperoxide	1.85 (cal)

Test substance	:	EP-306 Components
Conclusion	:	Components have a Log Ko/w between about –0.6 and 2
Reliability	:	(2) valid with restrictions EPIWIN estimates are assigned a reliability of 2
Flag	:	Critical study for SIDS endpoint

26.12.2003 (3,4)

2.6.1 WATER SOLUBILITY

Value :
pH Value : 2.4
concentration : 50 g/l at 20 °C
PKa :
Description : Miscible
Method : Determined via unknown method by BASF AG on product
Year :
GLP :
Test substance : Dicarbonsaeure Loesung A. Ber. Trocken
Reliability
26.12.2003 (2)

Value : 2,750 to 955,000 mg/l at 25 °C
pH Value :
concentration :
PKa :
Description :
Method : other (calculated): EPI Suite (v3.10)
Year :
GLP :
Test substance :

Method : EPI Suite (v3.10) was used to determine the water solubility of EP-306 components at 25 °C to gain an understanding of the components range of water solubilities. Calculations were based in CAS Nos.

Result :

Component	Water Sol (mg/L)
Formic Acid	955,000
Acetic Acid	476,000
Propionic Acid	174,000
Butyric Acid	66,100
Valeric Acid	18,600
Caproic Acid	5,900
Succinic Acid	808,000
Glutaric Acid	396,000
Adipic Acid	167,000
6-Hydroxycaproic Acid	229,000
Cyclohexanol	33,700
Cyclohexanone	24,100
Cyclohexyl Hydroperoxide	2,750

Test substance : EP-306 Components
Conclusion : The mixture can be considered soluble in water
Reliability : (2) valid with restrictions
EPIWIN estimates are assigned a reliability of 2
Flag : Critical study for SIDS endpoint
27.12.2003 (4)

3.1.1 PHOTODEGRADATION

Type	:	Air
Light Source	:	Sun light
Sensitizer	:	OH
Conc. of Sensitizer	:	1.5E6 OH/cm^3
Rate Constant	:	
Degradation	:	
Method	:	other (calculated): EPI Suite (v3.10)
Year	:	
GLP	:	
Test substance	:	

Method : The overall OH rate constant (cm3/molecule*sec) and half-life (days) for each EP-306 component was calculated with EPI Suite based on its CAS No. The table below provides a summary of these values..

Result :

EP-306 Component	OH Rate Constant (cm3/mol.*s)	Half-life (days)
Formic Acid	0.520×10^{-12}	20.6
Acetic Acid	0.622×10^{-12}	17.2
Propionic Acid	1.39×10^{-12}	7.71
Butyric Acid	2.70×10^{-12}	3.96
Valeric Acid	4.11×10^{-12}	2.60
Caproic Acid	5.52×10^{-12}	1.94
Succinic Acid	2.76×10^{-12}	3.87
Glutaric Acid	4.18×10^{-12}	2.56
Adipic Acid	5.59×10^{-12}	1.91
6-Hydroxycaproic Acid	9.78×10^{-12}	1.09
Cyclohexanol	17.5×10^{-12}	0.61
Cyclohexanone	12.1×10^{-12}	0.88
Cyclohexyl Hydroperoxide	14.0×10^{-12}	0.76

Test substance : EP-306 Components

Conclusion : Components have half-lives between about 0.6 and 20 days, with major components exhibiting half-lives of about 1 to 2 days.

Reliability : (2) valid with restrictions
EPIWIN estimates are assigned a reliability of 2

Flag : Critical study for SIDS endpoint

26.12.2003 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	other: water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	
Year	:	

Method : EP-306 components, when well mixed into the environment, will distribute according to their individual physical-chemical properties. To understand the relative distribution of components, it is necessary to look at the individual components. It was assumed that materials originated in water as this is considered the most likely manner in which EP-306 will enter the environment.

Result :

SMILES : O=CO
CHEM : Formic acid
CAS NUM: 000064-18-6
MOL FOR: C1 H2 O2
MOL WT : 46.03
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00633	570	0
Water	99.8	208	1000
Soil	0.021	208	0
Sediment	0.149	832	0

Persistence Time: 231 hr

****
SMILES : O=C(O)C
CHEM : Acetic acid
CAS NUM: 000064-19-7
MOL FOR: C2 H4 O2
MOL WT : 60.05
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0027	347	0
Water	99.8	208	1000
Soil	0.0149	208	0
Sediment	0.15	832	0

Persistence Time: 231 hr

****
SMILES : O=C(O)CC
CHEM : Propanoic acid
CAS NUM: 000079-09-4
MOL FOR: C3 H6 O2
MOL WT : 74.08
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0232	210	0
Water	99.8	208	1000
Soil	0.0294	208	0
Sediment	0.151	832	0

Persistence Time: 231 hr

****
SMILES : O=C(O)CCC
CHEM : Butanoic acid

CAS NUM: 000107-92-6
MOL FOR: C4 H8 O2
MOL WT : 88.11
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.025	107	0
Water	99.8	208	1000
Soil	0.0271	208	0
Sediment	0.156	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCCC
CHEM : Pentanoic acid
CAS NUM: 000109-52-4
MOL FOR: C5 H10 O2
MOL WT : 102.13
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0178	62.4	0
Water	99.8	208	1000
Soil	0.0233	208	0
Sediment	0.176	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCCCC
CHEM : Hexanoic acid
CAS NUM: 000142-62-1
MOL FOR: C6 H12 O2
MOL WT : 116.16
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0267	46.5	0
Water	99.7	208	1000
Soil	0.0237	208	0
Sediment	0.234	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCC(=O)O
CHEM : Butanedioic acid
CAS NUM: 000110-15-6
MOL FOR: C4 H6 O4
MOL WT : 118.09
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	5.34e-014	92.9	0
Water	99.9	208	1000

Soil	7.9e-008	208	0
Sediment	0.149	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCCC(=O)O
CHEM : Pentanedioic acid
CAS NUM: 000110-94-1
MOL FOR: C5 H8 O4
MOL WT : 132.12
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.37e-013	61.5	0
Water	99.9	208	1000
Soil	1.27e-007	208	0
Sediment	0.15	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCCCC(=O)O
CHEM : Hexanedioic acid
CAS NUM: 000124-04-9
MOL FOR: C6 H10 O4
MOL WT : 146.14
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	9.39e-012	45.9	0
Water	99.8	208	1000
Soil	1.05e-006	208	0
Sediment	0.15	832	0
Persistence Time:	231 hr		

****
SMILES : O=C(O)CCCCCO
CHEM : 6-HYDROXYCAPROIC ACID
CAS NUM: 001191-25-9
MOL FOR: C6 H12 O3
MOL WT : 132.16
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	7.52e-011	26.2	0
Water	99.8	208	1000
Soil	3.03e-006	208	0
Sediment	0.153	832	0
Persistence Time:	231 hr		

****
SMILES : OC(CCCC1)C1
CHEM : Cyclohexanol
CAS NUM: 000108-93-0
MOL FOR: C6 H12 O1

MOL WT : 100.16
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0757	14.7	0
Water	99.7	360	1000
Soil	0.0165	360	0
Sediment	0.19	1.44e+003	0

Persistence Time: 338 hr

****
SMILES : O=C(CCCC1)C1
CHEM : Cyclohexanone
CAS NUM: 000108-94-1
MOL FOR: C6 H10 O1
MOL WT : 98.15
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.315	40.2	0
Water	99.5	360	1000
Soil	0.0317	360	0
Sediment	0.175	1.44e+03	0

Persistence Time: 334 hr

****
SMILES : C1(OO)CCCCC1
CHEM :
CAS NUM: 000766-07-4
MOL FOR: C6 H12 O2
MOL WT : 116.16
---------- EPI SUMMARY (v3.10) ----------
Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.248	18.3	0
Water	99.5	360	1000
Soil	0.0232	360	0
Sediment	0.262	1.44e+03	0

Persistence Time: 330 hr

Test substance : EP-306 Components
Conclusion : EP-306 compounds if released into water, will distribute primarily to water.
Reliability : (2) valid with restrictions
Calculated values are assigned a reliability of 2.
Flag : Critical study for SIDS endpoint
26.10.2003 (6)

3.5 BIODEGRADATION

Type : Aerobic
Inoculum : activated sludge, domestic
Concentration : 65 mg/l

Contact time	:	
Degradation	:	= 70 - 80 % after 28 days
GLP	:	Yes
Year	:	1992
Result	:	Biodegradable
Method	:	CO_2 Evolution Test preformed according to the OECD-301B test guideline
Result	:	Evolution of CO_2 from the test material reached 52% of the theoretical CO_2 content ($ThCO_2$) at 14 days and 78% at 28 days. The CO_2 / $ThCO_2$ value for the reference substance (aniline) was 60% - 70% at 14 days.
Test condition	:	The test substance concentration and total organic carbon concentration were 65 mg/l and 20 mg/l, respectively. Inoculum consisted of activated sludge from laboratory waste treatment plants which were fed with municipal and synthetic sewage. Sludge was washed for 24 hours and then added to test vessels at a concentration of 30 mg/l dry solids.
Test substance	:	Dicarboxylic acid solution: water (42.9%), free carboxylic acids (27.8%), and alcohols (13.3%)
Reliability	:	(1) valid without restrictions GLP guideline study.

26.12.2003 (7)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static
Species : *Leuciscus idus L.,* golden variety (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 215 nominal
LC0 : 215 nominal
LC50 : 215 - 464 nominal
Limit test : No
Analytical monitoring : No
Method : DIN 38 412
Year :
GLP : No
Test substance :

Method : After preliminary tests, 10 fish (golden orfe, mean wt 2.8 g) were exposed to test material at one of four concentrations. Glass test containers (16 l) contained 10 liters of demineralized tap water resalted with: 294.0 mg/l $CaCl_2 \bullet 2\ H_20$, 123.3 mg/l $MgSO_4 \bullet 7\ H_20$, 64.8 mg/l NaHCO3, and 5.8 mg/l KCl. Test material was added directly to the vessels without pretreatment. Ten fish were added to each container after the test material had been mixed with the test water.

Conditions were:

Temperature	20 °C
Acid Capacity	0.8 mmol/l
Total Hardness	2.5 mmol/l
Ratio Ca/Mg Ions	4
Ratio Na/K Ions	10
pH	~7.9 (control)
DOC	(see table)

Remark :
Result : In the definitive test, the following results were recorded

Nom. Conc		No. Dead Fish at					
(mg/L)	# fish	1 hr	4 hr	24 hr	48 hr	72 hr	96 hr
100	10	0	0	0	0	0	0
215	10	0	0	0	0	0	0
464	10	0	1*	9*	10	10	10
1000	10	0*	1	10	10	10	10
0	10	0	0	0	0	0	0
1000**	10	0	0	0	0	0	0

* Symptoms: Narcotic-like state
** Test solution after pH-adjustment

Nom. Conc		pH at			
(mg/L)	Start	24 hr	48 hr	72 hr	96 hr
100	7.2	7.7	7.6	7.7	7.7
215	5.8	6.4	6.9	7.2	7.3
464	4.7	4.9	4.9		
1000	4.2				

0	8.0	7.9	7.8	7.9	7.9
1000**	7.3	7.7	7.7	7.7	7.7

** Test solution after pH-adjustment

Nom. Conc	Oxygen Content (mg/l) at				
(mg/L)	Start	24 hr	48 hr	72 hr	96 hr
100	8.2	8.2	8.2	8.3	8.4
215	8.3	7.8	7.7	7.8	7.9
464	8.4	8.8	7.7		
1000	8.7				
0	8.0	8.3	8.2	8.1	8.2
1000**	8.3	8.5	8.3	8.2	8.1

** Test solution after pH-adjustment

Test substance : Dicarbonsaeureloesung L. Ber. Trocken
Conclusion : The LC50 for the golden orfe under these conditions is 215 - 464 mg/L.
Reliability : (1) valid without restriction
Well-documented guideline study conducted under GLP-like conditions. Comparable to OECD 203 study except for test species.
Flag : Critical study for SIDS endpoint
30.12.2003 (8)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static
Species : *Daphnia magna* (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : > 100 (nominal)
EC50 : > 100 (nominal)
24 hour EC50 : > 100 (nominal)
Limit Test : no
Analytical monitoring : Yes
Method : Acute toxicity for Daphnia. EEC Directive 79/831/EEC, Annex V, Part C2.
Year : 1989
GLP : Yes

Method : A static toxicity test was conducted in 20 mL test tubes containing 10 mL test solution. The dilution water used in this study was an ultrapure, deionized water (conductivity < 0.05 µS/cm) containing the following macronutrients (mg/l): Ca (80.1), Mg (12.2), Na (19.8), K (3.2), Si (1.0), Cl (144.9), NO_3 (0.2), PO_4 (0.2), SO_4 (48.4), HCO_3 (47.1) and vitamins (µg/l): thiamine (75.0), B_{12} (1.0), biotin (0.75). The medium had the following properties:

Temperature	20 ± 2 °C
Alkalinity up to pH 4.3	0.80 – 1.00 mmol/l
Total Hardness	2.20 – 3.20 mmol/l
Ratio Ca/Mg Ions	~4
pH	7.5 – 8.5
Conductivity	550 – 650 µS/cm

Test solutions were made by the combining the dilution water with the test material to yield concentrations (mg/l) of: 0, 12.5, 25, 50, 100. Twenty *daphnids* (5 per test tube; 4 test tubes per concentration) were exposed to each test solution. *Daphnid* swimming ability was evaluated at 0, 3, 24, and 48 hr after gentle agitation of the test tube

Temperature was measured at 0, 24, and 48 hr in a extra test tube close to the experimental test tubes; temperatures ranged from 20.3 °C – 21.5 °C. Oxygen content and pH were measured at 0 and 48 hr in one replicate of each test concentration; results are provided below.

Nom. Conc	pH		Oxygen Content (mg/l)	
(mg/L)	0 hr	48 hr	0 hr	48 hr
0	8.0	7.9	8.4	8.3
12.5	7.8	7.8	8.4	7.5
25	7.5	7.8	8.2	7.3
50	7.2	7.6	8.2	7.4
100	6.6	7.4	8.2	7.3

Analayses were performed at 0 hr and 48 hr using the 6-hydroxyhexanoic acid peak for quantification. Results are provided below.

Nom. Conc	Measured concentration (mg/l)(% Nominal)		
(mg/L)	0 hr	48 hr (- daphnids)	48 hr (+ daphnids)
0	< 5 (100)	< 5 (100)	< 5 (100)
12.5	14 (117)	15 (120)	12 (96)
100	97 (97)	130 (130)	146 (146)

Result : *Daphnid* swimming ability was not affected at any of the times or concentrations evaluated. Test material recovery rate at 48 hr ranged from 100 – 150%.

Test substance : Dicarboxylic acid solution. Product No. 3265 (Basant); Batch No. 849-2-PRST-71.

Conclusion : The 48 hours EC50 was > 100 mg/L

Reliability : (1) valid without restriction
Well-documented, guideline study

Flag : Critical study for SIDS endpoint

30.12.2003 (9)

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : > 5000 mg/kg bw
Species : Rat
Strain : Wistar
Sex : male/female
Number of animals :
Vehicle : other: Dosed neat
Doses : 681, 2150, 3160, and 5000 mg/kg bw
Method :
Year :
GLP : No
Test substance :

Method : Rats were housed at 22 ± 2 °C, 30% - 70% relative humidy and a 12-hr on / 12-hr off light cycle. Test substance was diluted with distilled water and administered to Wistar rats by gavage at a volume of 10 ml/kg. Treated animals (5 males/5 females per group) were observed for 21 days; survivors were sacrificed and subjected to a gross pathological examination. Mean body weights were reported at the time of dosing and at 7, 13 and 21 days post-dosing.

Remark :
Result :

Dose (mg/kg)	Deaths (M = male, F = female)
681	No Deaths
2150	1M (day 21), 1F (day 1)
3160	1F (day 14)
5000	1M (day 7), 2F (days 7, 14)

Dose (mg/kg)	Mean Male Body Weight (g)			
	Start	Day 7	Day 13	Day 20
681	188	258	296	330
2150	188	249	270	326
3160	191	264	298	332
5000	181	218	253	282

Dose (mg/kg)	Mean Female Body Weight (g)			
	Start	Day 7	Day 13	Day 20
681	172	200	210	218
2150	181	217	226	240
3160	188	205	228	239
5000	190	196	225	230

Male Symptoms	Dose (mg/kg)			
	681	2150	3160	5000
Dyspnea	---	1D – 2D	1D - 2D	1D – 14D
Apathy	---	---	!D - 2D	1D – 14D
Staggering	---	1D – 2D	1D - 2D	4D – 15D
Spastic Gait	---	---	---	14D – 15D
Piloerection	---	1D – 2D	1D - 2D	1D – 15D
Impaired General State	---	1D – 2D	---	15D
Poor General State	---	---	1D - 2D	1D – 14D

Female Symptoms	Dose (mg/kg)			
	681	2150	3160	5000
Dyspnea	---	1D – 2D	4H - 2D	1D – 13D
Apathy	---	1D – 2D	4H - 2D	1D – 13D
Staggering	---	1D – 2D	4H - 2D	---
Piloerection	---	1D – 2D	4H - 2D	1D – 15D
Poor General State	---	1D – 2D	4H - 2D	1D – 13D

No abnormalities were noted at necropsy.

Test substance : Abstreifsaeure
Conclusion : The Oral LD50 is greater than 5,000 mg/kg in Wistar rats of each sex.
Reliability : (1) valid without restrictions
Procedure equivalent to OECD 401. Good documentation for an older study.

30.12.2003 (10)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : *Salmonella typhimurium*, Reverse Mutation Assay
System of testing : Reverse mutation, plate incorporation and preincubation methods
Test concentration : 40, 200, 1000, 5000 and 10,000 µg/plate
Cycotoxic concentr. : ≥ 5,000 µg/plate
Metabolic activation : with and without
Result : Negative
Method : OECD 471
Year :
GLP : Yes
Test substance :

Method : The mutagenic potential of dicarboxylic acid solution (DAS) was evaluated using the *S. typhimurium* strains TA1535, TA1537, TA98, and TA100 with and without metabolic activation (S-9). The homogeneity of the test substance was assured by melting at 70 °C and mixing prior to preparation of the test solutions. No test substance precipitation was observed in the studies. Tester strains were exposed according to the direct plate incorporation and preincubation methods. Liver microsomal fractions from male Sprague-Dawley rats (200 - 300 g) were prepared according to established methods. The positive control with S-9 mix was 2-aminoanthracene (dissolved in DMSO) for all 4 strains; positive controls without S-9 mix included: N-methyl-N'-nitro-N-nitrosoguanidine (in DMSO) for TA 100 and TA 1535, 4-nitro-o-phenyldiamine (in DMSO) for TA 98, and 9-aminoacridine chloride monohydrate (in DMSO) for TA 1537. Negative controls were exposed to DMSO only. DAS was dissolved in DMSO and tested at concentrations of 40, 200, 1000, 5000, and 10000 µg/plate. Assays were performed in two independent experiments, using identical procedures, both with and without metabolic activation. Each concentration, including the controls, was tested in triplicate.

In general, positive substances were required to demonstrate (a) doubling of the spontaneous mutation rate, (b) dose-response relationship, and (c) reproducibility of results.

Remark : Test dates: Standard Plate (13-Aug-1996); Preincubation (12-Sep-1996)
Result : Both the direct plate and preincubation assays demonstrated a lack of mutagenic activity DAS. No significant increases in the number of

revertants were found in any strain and DAS treatment group combination relative to the solvent control. In addition, no concentration-dependent enhancement of the revertant number occurred, and no differences were observed between DAS treatments with or without metabolic activation.

Test substance : Dicarboxylic acid solution, batch No. VN-5200, manufactured on 21-Feb-1996.

Reliability : (1) valid without restrictions
GLP guideline study

30.12.2003 (11)

Type : *Escherichia coli*, Reverse Mutation Assay
System of testing : Reverse mutation, plate incorporation and preincubation methods
Test concentration : 40, 200, 1000, 5000 and 10,000 μg/plate
Cycotoxic concentr. : ≥ 5,000 μg/plate
Metabolic activation : with and without
Result : Negative
Method : OECD 472
Year :
GLP : Yes
Test substance :

Method : The mutagenic potential of dicarboxylic acid solution (DAS) was evaluated using the *E. coli* strain WP2 uvrA with and without metabolic activation (S-9). The homogeneity of the test substance was assured by melting at 70 °C and mixing prior to preparation of the test solutions. No test substance precipitation was observed in the studies. The tester strain was exposed according to the direct plate incorporation and preincubation methods. Liver microsomal fractions from male Sprague-Dawley rats (200 - 300 g) were prepared according to established methods. The positive control with S-9 mix was 2-aminoanthracene (dissolved in DMSO); the positive control without S-9 mix was N-ethyl-N'-nitro-N-nitrosoguanidine (in DMSO). Negative controls were exposed to DMSO only. DAS was dissolved in DMSO and tested at concentrations of 40, 200, 1000, 5000, and 10000 μg/plate. Assays were performed in two independent experiments, using identical procedures, both with and without metabolic activation. Each concentration, including the controls, was tested in triplicate.

In general, positive substances were required to demonstrate (a) doubling of the spontaneous mutation rate, (b) dose-response relationship, and (c) reproducibility of results.

Remark : Test dates: Standard Plate (13-Aug-1996); Preincubation (12-Sep-1996)

Result : Both the direct plate and preincubation assays demonstrated a lack of mutagenic activity DAS. No significant increases in the number of revertants were found in any strain and DAS treatment group combination relative to the solvent control. In addition, no concentration-dependent enhancement of the revertant number occurred, and no differences were observed between DAS treatments with or without metabolic activation.

Test substance : Dicarboxylic acid solution, batch No. VN-5200, manufactured on 21 February 1996.

Reliability : (1) valid without restrictions
GLP guideline study

30.12.2003 (11)

(1) BASF Corporation Technical Bulletin. EP-306 Acid Water. February 1997

(2) BASF Aktiengesellschaft Safety Data Sheet. Dicarbonsaeure Loesung A. Ber Trocken. Revised December 15, 2003

(3) EPI Suite (v3.10). KOWWIN (v1.66). USEPA Office of Pollution Prevention and Toxics and Syracuse Research Corporation (April 2001)

(4) EPI Suite (v3.10). WSKOW (v1.40). USEPA Office of Pollution Prevention and Toxics and Syracuse Research Corporation (April 2001)

(5) EPI Suite (v3.10). AOP Program (v1.90). USEPA Office of Pollution Prevention and Toxics and Syracuse Research Corporation (April 2001)

(6) EPI Suite (v3.10). Level III Fugacity Model. USEPA Office of Pollution Prevention and Toxics and Syracuse Research Corporation (April 2001)

(7) BASF Aktiengesellschaft. 10 December 1997. Determination of the biodegradability of dicarboxylic acid solution in the co2-evolution test. Project No.: 97/0071/22/1.

(8) BASF Aktiengesellschaft. 2 December 1987. Report on the study of the acute toxicity of dicarbonsaeureloesung L. Ber. Trocken on the golden orfe (Leuciscus idus L., golden variety). Project No.: 10F0220/875098

(9) BASF Aktiengesellschaft. 18 December 1997. Determination of the acute effect of dicarboxylic acid solution on the swimming ability of the water flea *Daphnia magna Straus*. Project No.: 97/0071/50/1

(10) BASF Aktiengesellschaft. 9 November 1987. Report on the study of acute oral toxicity of abstreifsaeure in the rat. Project No.: 10A0220/871107.

(11) BASF Aktiengesellschaft. 5 May 1998. Report on the study of Dicarbonsaeure-Loesung in the Ames *Salmonella* / mammalian-microsome mutagenicity test and *Escherichia coli* / mammalian-microsome reverese mutation assay (standard plate test and preincubation test). Project No.: 40M0135/964062